

## Author Index to Volume 153

- |   |                |
|---|----------------|
| Abascal, J.L.F. and P. Turq, Cluster structure in model electrolyte solutions   | 153 (1991) 79  |
| Abramson, E., see P. Dupré  | 153 (1991) 539 |
| Achiba, Y., see Y. Luo  | 153 (1991) 473 |
| Adamowicz, L., see A. Leś   | 153 (1991) 409 |
| Ågren, H., see Y. Luo   | 153 (1991) 473 |
| Alper, J.S., H. Dothe and D.F. Coker, Vibrational structure of the solvated glycine zwitterion  | 153 (1991) 51  |
| André, B., see J.-Y. Moisan   | 153 (1991) 305 |
| André, B., see J.Y. Moisan  | 153 (1991) 465 |
| Andrew, J.J., D.C. McDermott, S.P. Mills and C.J.S.M. Simpson, Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon  | 153 (1991) 247 |
| Archirel, P., see N. Levasseur  | 153 (1991) 387 |
| Bagryanskaya, E.G., see I.A. Shkrob   | 153 (1991) 427 |
| Barnett, S.M., N.J. Mason and W.R. Newell, Production of the $N_2(A^3\Sigma^+_u)$ metastable state by electron impact dissociative excitation of $N_2O$   | 153 (1991) 283 |
| Barzoukas, M., A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud, Conformational dependence of the quadratic hyperpolarisabilities of a series of push-pull diaryl acetylenes: an experimental and computational investigation | 153 (1991) 457 |
| Bauschlicher Jr., C.W., see S.R. Langhoff   | 153 (1991) 1   |
| Bauschlicher Jr., C.W., see K. Faegri Jr.   | 153 (1991) 399 |
| Boeglin, A., see M. Barzoukas   | 153 (1991) 457 |
| Brion, C.E., see W. Zhang   | 153 (1991) 491 |
| Buchachenko, A.L., see I.A. Shkrob  | 153 (1991) 443 |
| Bzenic, S.A., see S.B. Vrhovac  | 153 (1991) 233 |
| Caballol, R., see J. Miralles   | 153 (1991) 25  |
| Cai, M., see M.B. Partenskii  | 153 (1991) 125 |
| Carman, B., see Y. Luo  | 153 (1991) 473 |
| Cartwright, D.C., P.J. Hay and S. Trajmar, Estimation of the integral cross section for dissociative excitation of $F_2$ by electron impact   | 153 (1991) 219 |
| Cheng, Y.D., see Y. Luo   | 153 (1991) 473 |
| Coker, D.F., see J.S. Alper   | 153 (1991) 51  |
| Cooper, G., see W. Zhang  | 153 (1991) 491 |
| Costes, M., see C. Naulin   | 153 (1991) 519 |
| Datta, A., see S. Ghoshal   | 153 (1991) 161 |
| Delhalle, J., see M. Raynaud  | 153 (1991) 39  |
| Desouter-Lecomte, M., see F. Remacle  | 153 (1991) 201 |
| Diehl, F., see K. Kesper  | 153 (1991) 511 |
| Dietz, F., see T. Krossner  | 153 (1991) 63  |

## Author Index to Volume 153

- Abascal, J.L.F. and P. Turq, Cluster structure in model electrolyte solutions 153 (1991) 79
- Abramson, E., see P. Dupré 153 (1991) 539
- Achiba, Y., see Y. Luo 153 (1991) 473
- Adamowicz, L., see A. Leś 153 (1991) 409
- Ågren, H., see Y. Luo 153 (1991) 473
- Alper, J.S., H. Dothe and D.F. Coker, Vibrational structure of the solvated glycine zwitterion 153 (1991) 51
- André, B., see J.-Y. Moisan 153 (1991) 305
- André, B., see J.Y. Moisan 153 (1991) 465
- Andrew, J.J., D.C. McDermott, S.P. Mills and C.J.S.M. Simpson, Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon 153 (1991) 247
- Archirel, P., see N. Levasseur 153 (1991) 387
- Bagryanskaya, E.G., see I.A. Shkrob 153 (1991) 427
- Barnett, S.M., N.J. Mason and W.R. Newell, Production of the  $N_2$  ( $A^3\Sigma^+_u$ ) metastable state by electron impact dissociative excitation of  $N_2O$  153 (1991) 283
- Barzoukas, M., A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud, Conformational dependence of the quadratic hyperpolarisabilities of a series of push-pull diaryl acetylenes: an experimental and computational investigation 153 (1991) 457
- Bauschlicher Jr., C.W., see S.R. Langhoff 153 (1991) 1
- Bauschlicher Jr., C.W., see K. Faegri Jr. 153 (1991) 399
- Boeglin, A., see M. Barzoukas 153 (1991) 457
- Brion, C.E., see W. Zhang 153 (1991) 491
- Buchachenko, A.L., see I.A. Shkrob 153 (1991) 443
- Bzenic, S.A., see S.B. Vrhovac 153 (1991) 233
- Caballol, R., see J. Miralles 153 (1991) 25
- Cai, M., see M.B. Partenskii 153 (1991) 125
- Carman, B., see Y. Luo 153 (1991) 473
- Cartwright, D.C., P.J. Hay and S. Trajmar, Estimation of the integral cross section for dissociative excitation of  $F_2$  by electron impact 153 (1991) 219
- Cheng, Y.D., see Y. Luo 153 (1991) 473
- Coker, D.F., see J.S. Alper 153 (1991) 51
- Cooper, G., see W. Zhang 153 (1991) 491
- Costes, M., see C. Naulin 153 (1991) 519
- Datta, A., see S. Ghoshal 153 (1991) 161
- Delhalle, J., see M. Raynaud 153 (1991) 39
- Desouter-Lecomte, M., see F. Remacle 153 (1991) 201
- Diehl, F., see K. Kesper 153 (1991) 511
- Dietz, F., see T. Krossner 153 (1991) 63

- Doktorov, A.B., see V.A. Morozov 153 (1991) 313
- Doktorov, A.B., see V.A. Morozov 153 (1991) 333
- Dorthe, G., see C. Naulin 153 (1991) 519
- Dothe, H., see J.S. Alper 153 (1991) 51
- Dupré, P., R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field, Anomalous behaviour of the anticrossing density as a function of excitation energy in the C<sub>2</sub>H<sub>2</sub> molecule, *Chem. Phys.* 152 (1991) 293. Erratum 153 (1991) 539
- Ejeklint, P., see Y. Luo 153 (1991) 473
- Ellinger, Y., see M. Raynaud 153 (1991) 39
- Faegri Jr., K. and C.W. Bauschlicher Jr., Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd 153 (1991) 399
- Ferrari, L., Heavy ions in mixtures of light gases: Fokker-Planck equation and its solution 153 (1991) 115
- Feulner, P., see R. Treichler 153 (1991) 259
- Field, R.W., see P. Dupré 153 (1991) 539
- Fink, E.H., see A.F. Vilesov 153 (1991) 531
- Fort, A., see M. Barzoukas 153 (1991) 457
- Fotakis, C., see E. Patsilnakou 153 (1991) 503
- Galasso, V., Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spirononaterene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene 153 (1991) 13
- Ghelichkhani, E. and E.R. Grant, On the Jahn-Teller coupling of an orbital triplet with a vibrational doublet 153 (1991) 133
- Ghoshal, S. and A. Datta, Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump 153 (1991) 161
- Grant, E.R., see E. Ghelichkhani 153 (1991) 133
- Green, P.G., see P. Dupré 153 (1991) 539
- Hay, P.J., see D.C. Cartwright 153 (1991) 219
- Hennico, G., see M. Raynaud 153 (1991) 39
- Ibuki, T., see W. Zhang 153 (1991) 491
- Jelenkovic, B.M., see S.B. Vrhovac 153 (1991) 233
- Jordan, P.C., see M.B. Partenskii 153 (1991) 125
- Jost, R., see P. Dupré 153 (1991) 539
- Kesper, K., F. Diehl, J.G.G. Simon, H. Specht and A. Schweig, Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation 153 (1991) 511
- Klein, G., see M. Barzoukas 153 (1991) 457
- Koutselos, A.D. and E.A. Mason, Generalized Einstein relations for ions in molecular gases 153 (1991) 351
- Krossner, T. and F. Dietz, A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines 153 (1991) 63

- Kudo, T. and S. Nagase, The structures and stability of the  $\text{Si}_3\text{H}_6^{2+}$  dications. A theoretical study 153 (1991) 379
- Lakhno, V.D. and O.V. Vasil'ev, The solvated electron in an electrolyte solution 153 (1991) 147
- Langhoff, S.R., H. Partridge and C.W. Bauschlicher Jr., Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO 153 (1991) 1
- Leś, A. and L. Adamowicz, The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine 153 (1991) 409
- Levasseur, N., Ph. Millie, P. Archirel and B. Levy, Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the  $\text{CO}^{2+}$  case 153 (1991) 387
- Lever, R., see J.-Y. Moisan 153 (1991) 305
- Lever, R., see J.Y. Moisan 153 (1991) 465
- Levy, B., see N. Levasseur 153 (1991) 387
- Lombardi, M., see P. Dupré 153 (1991) 539
- Lorquet, J.C., see F. Remacle 153 (1991) 201
- Luo, Y., Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn, Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy 153 (1991) 473
- Malrieu, J.-P., see J. Miralles 153 (1991) 25
- March, N.H., see A. Nagy 153 (1991) 141
- Maripuu, R., see Y. Luo 153 (1991) 473
- Martin, M.M., P. Plaza and Y.H. Meyer, Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation 153 (1991) 297
- Mason, E.A., see A.D. Koutselos 153 (1991) 351
- Mason, N.J., see S.M. Barnett 153 (1991) 283
- McDermott, D.C., see J.J. Andrew 153 (1991) 247
- McKee, M.L., see M.R. Soto 153 (1991) 415
- Mendaš, I. and P. Milutinović, Trajectory capture rate coefficients for ion-quadrupolar molecule reactions 153 (1991) 73
- Menzel, D., see R. Treichler 153 (1991) 259
- Meyer, Y.H., see M.M. Martin 153 (1991) 297
- Millie, Ph., see N. Levasseur 153 (1991) 387
- Mills, S.P., see J.J. Andrew 153 (1991) 247
- Milutinović, P., see I. Mendaš 153 (1991) 73
- Miralles, J., R. Caballol and J.-P. Malrieu, Observable-dedicated molecular orbitals.  
I. Method and illustrations 153 (1991) 25
- Misurkin, I.A., see A.L. Tchougreeff 153 (1991) 371
- Moisan, J.-Y., B. André and R. Lever, Xerographic dark discharge of PVK:TNF photoconductive material 153 (1991) 305
- Moisan, J.Y., B. André, R. Lever and C. Servens, Xerographic discharge of organic thermoplastic material 153 (1991) 465
- Morozov, V.A. and A.B. Doktorov, Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field 153 (1991) 313
- Morozov, V.A. and A.B. Doktorov, Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field 153 (1991) 333

- Nagase, S., see T. Kudo 153 (1991) 379
- Nagy, A. and N.H. March, Relation between total energy and sum of orbital energies for neutral atoms 153 (1991) 141
- Naulin, C., M. Costes and G. Dorthe, The  $C(^3P_r) + NO(X^2\Pi_r) \rightarrow CN(X^2\Sigma^+) + O(^3P_r)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams 153 (1991) 519
- Newell, W.R., see S.M. Barnett 153 (1991) 283
- Nicoud, J.F., see M. Barzoukas 153 (1991) 457
- Oddershede, J., see S.P.A. Sauer 153 (1991) 189
- Ogryzlo, E.A., see Z.H. Walker 153 (1991) 483
- Öhlund, L., see Y. Luo 153 (1991) 473
- Oswald, L., see M. Barzoukas 153 (1991) 457
- Page, M., see M.R. Soto 153 (1991) 415
- Palmer, M.H., see I.C. Walker 153 (1991) 169
- Partenskii, M.B., M. Cai and P.C. Jordan, A dipolar chain model for the electrostatics of transmembrane ion channels 153 (1991) 125
- Partridge, H., see S.R. Langhoff 153 (1991) 1
- Patsilinakou, E., D. Proch and C. Fotakis, Multiphoton dissociation dynamics of highly excited states of  $CS_2$  and  $CS_2$  clusters 153 (1991) 503
- Petrovic, Z.Lj., see S.B. Vrhovac 153 (1991) 233
- Plaza, P., see M.M. Martin 153 (1991) 297
- Polák, R., An extended diatomics-in-molecules model for  $NH_2^+$  153 (1991) 91
- Proch, D., see E. Patsilinakou 153 (1991) 503
- Radovanov, S.B., see S.B. Vrhovac 153 (1991) 233
- Raynaud, M., C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle, Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition 153 (1991) 39
- Remacle, F., M. Desouter-Lecomte and J.C. Lorquet, Quantum effects in competitive unimolecular reactions 153 (1991) 201
- Reynaud, C., see M. Raynaud 153 (1991) 39
- Riedl, W., see R. Treichler 153 (1991) 259
- Sauer, S.P.A., V. Špirko and J. Oddershede, The magnetizability and *g*-factor surfaces of ammonia 153 (1991) 189
- Schweig, A., see K. Kesper 153 (1991) 511
- Seibt, W., see Y. Luo 153 (1991) 473
- Serbutoviez, C., see M. Barzoukas 153 (1991) 457
- Servens, C., see J.Y. Moisan 153 (1991) 465
- Shkrob, I.A., V.F. Tarasov and E.G. Bagryanskaya, Electron spin exchange in micellized radical pairs. I.  $^{13}C$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}C$  radio frequency stimulated nuclear polarization (SNP) 153 (1991) 427
- Shkrob, I.A., V.F. Tarasov and A.L. Buchachenko, Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs 153 (1991) 443
- Siegbahn, K., see Y. Luo 153 (1991) 473
- Simon, J.G.G., see K. Kesper 153 (1991) 511
- Simpson, C.J.S.M., see J.J. Andrew 153 (1991) 247

- Soto, M.R., M. Page and M.L. McKee, Theoretical study of the reaction of OH with HNO 153 (1991) 415  
Specht, H., see K. Kesper 153 (1991) 511  
Špirko, V., see S.P.A. Sauer 153 (1991) 189  
Storozhev, A.V. and M.L. Strekalov, Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation 153 (1991) 99  
Strekalov, M.L., see A.V. Storozhev 153 (1991) 99  
  
Tarasov, V.F., see I.A. Shkrob 153 (1991) 427  
Tarasov, V.F., see I.A. Shkrob 153 (1991) 443  
Tchougreeff, A.L. and I.A. Misurkin, Ferromagnetism of charge-transfer crystals 153 (1991) 371  
Trajmar, S., see D.C. Cartwright 153 (1991) 219  
Treichler, R., W. Wurth, W. Riedl, P. Feulner and D. Menzel, Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces 153 (1991) 259  
Turq, P., see J.L.F. Abascal 153 (1991) 79  
  
Vasil'ev, O.V., see V.D. Lakhno 153 (1991) 147  
Vilesov, A.F., J. Wildt and E.H. Fink, Emission of Xe:N(<sup>2</sup>P) collision complexes near the N(<sup>2</sup>P→<sup>2</sup>D) lines 153 (1991) 531  
Vrhovac, S.B., S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković, Dissociative excitation of hydrogen in rf and dc glow discharges through H<sub>2</sub> 153 (1991) 233  
  
Walker, I.C. and M.H. Palmer, The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations 153 (1991) 169  
Walker, Z.H. and E.A. Ogryzlo, Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine 153 (1991) 483  
Wildt, J., see A.F. Vilesov 153 (1991) 531  
Wurth, W., see R. Treichler 153 (1991) 259  
  
Xing, K.Z., see Y. Luo 153 (1991) 473  
  
Zhang, W., G. Cooper, T. Ibuki and C.E. Brion, Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of CFCI<sub>3</sub> 153 (1991) 491

# List of Subjects

## 1 Methods

### 1.1 Theoretical

- 1.1.1 Group theory and algebras
- 1.1.2 Classical mechanics \*
- 1.1.3 Quantized field theory
- 1.1.4 Many body and quasiparticle approaches \*
- 1.1.5 Coupling schemes and perturbative treatments \*
- 1.1.6 Relativistic quantum mechanics
- 1.1.7 Transport quantum mechanics
- 1.1.8 Equilibrium statistical mechanics \*
- 1.1.9 Statistical mechanics of stationary states \*
- 1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories \*
- 1.1.11 Ab initio schemes for stationary properties \*
- 1.1.12 Computational and simulation methods \*
- 1.1.13 Molecular dynamics and scattering theory \*

### 1.2 Experimental

- 1.2.1 Magnetic resonances \*
- 1.2.2 Cyclotron resonance
- 1.2.3 Microwave spectroscopy \*
- 1.2.4 Infrared spectroscopy
- 1.2.5 Raman spectroscopy
- 1.2.6 Visible and UV spectroscopy \*
- 1.2.7 Fluorescence spectroscopy \*
- 1.2.8 Photoelectron and Auger spectroscopy \*
- 1.2.9 X-ray spectroscopy
- 1.2.10 Electron impact spectroscopy \*
- 1.2.11 Laser methods \*
- 1.2.12 Picosecond spectroscopy \*
- 1.2.13 Non-linear optical spectroscopy \*
- 1.2.14 Synchrotron spectroscopies \*
- 1.2.15 Coherent optical spectroscopy
- 1.2.16 Optical pumping
- 1.2.17 Multiple resonance spectroscopy
- 1.2.18 Optoacoustic spectroscopy
- 1.2.19 Atomic and molecular beam techniques
- 1.2.20 Time-resolved experiments \*
- 1.2.21 Mass spectrometry \*
- 1.2.22 Radiolysis
- 1.2.23 Mössbauer spectroscopy
- 1.2.24 X-ray, electron and neutron diffraction
- 1.2.25 Neutron scattering
- 1.2.26 Light scattering
- 1.2.27 Field emission and field ionization
- 1.2.28 Measurement of macroscopic variables \*

## 2 Objects

### 2.1 Bulk systems

- 2.1.1 Gases \*
- 2.1.2 Supersonic beams \*
- 2.1.3 Liquids neat
- 2.1.4 Liquid mixtures and solutions \*
- 2.1.5 Crystals \*
- 2.1.5.1 neat
- 2.1.5.2 mixed \*
- 2.1.6 Glasses
- 2.1.7 Liquid crystals
- 2.1.8 Polymers \*
- 2.1.9 Semiconductors \*
- 2.1.10 Metals and alloys
- 2.1.11 Thin films
- 2.1.12 Surfaces \*
- 2.1.13 Low-dimensional materials \*
- 2.1.14 Dielectrics \*
- 2.1.15 Plasmas \*
- 2.1.16 Biological systems \*

### 2.2 Microscopic systems

- 2.2.1 Atoms \*
- 2.2.2 Molecules (neutral and ionic) \*
- 2.2.2.1 diatomic \*
- 2.2.2.2 small polyatomics \*
- 2.2.2.3 aromatics \*
- 2.2.2.4 other large \*
- 2.2.2.5 polymeric and biological
- 2.2.3 Molecular aggregates \*
- 2.2.3.1 dimers \*
- 2.2.3.2 van der Waals molecules
- 2.2.3.3 clusters
- 2.2.3.4 complexes
- 2.2.4 Free radicals (including hydronium and muonium) \*
- 2.2.5 Quasiparticles (including excitons) \*
- 2.2.6 Defects and impurities \*
- 2.2.7 Ions and charge carriers \*

\* Denotes subjects covered in this volume



### 3 Phenomena

- 3.1 Molecular structure \*
- 3.2 Vibrations and rotations of molecules \*
- 3.3 Electronic structure and states \*
- 3.4 Electric and magnetic properties \*
- 3.5 Spin splittings
- 3.6 Optical activity
- 3.7 Molecular interactions \*
- 3.8 Spectral bandshapes and intensities \*
- 3.9 Coupling of electronic and nuclear motion \*
- 3.10 Energy transfer processes \*
- 3.11 Molecular photophysical processes \*
- 3.12 Intramolecular dynamics \*
- 3.12.1 radiationless transitions
- 3.12.2 vibrational energy redistribution (including vibrational dissociation) \*
- 3.13 Luminescence spectra, yields and lifetimes \*
- 3.14 Coherence loss processes
- 3.15 Non-linear responses (including optical) \*
- 3.16 Multiphoton phenomena \*
- 3.17 Reactions (including dissociation) \*
- 3.17.1 gas phase \*
- 3.17.2 condensed phase \*
- 3.17.3 photochemical \*
- 3.18 Tunnelling
- 3.19 Electron transfer \*
- 3.20 Positron annihilation
- 3.21 Ionization (including Rydberg states) \*
- 3.22 Molecular motion (including diffusive)
- 3.23 Isotopic effects
- 3.24 Fluctuations and noise
- 3.25 Collective motion and excitations
- 3.26 Surface effects and catalysis \*
- 3.27 Thermodynamic and transport properties \*
- 3.28 Structure of solids and liquids \*
- 3.29 Critical phenomena
- 3.30 Phase transitions \*



## Subject Index to Volume 153

### Methods

#### Theoretical

##### *Classical mechanics*

- Trajectory capture rate coefficients for ion-quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73

##### *Many body and quasiparticle approaches*

- The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147  
 Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371

##### *Coupling schemes and perturbative treatments*

- On the Jahn-Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133  
 Relation between total energy and sum of orbital energies for neutral atoms, A. Nagy and N.H. March 153 (1991) 141  
 Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161  
 Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313  
 Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333  
 Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

##### *Equilibrium statistical mechanics*

- Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79  
 A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125  
 Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161

##### *Statistical mechanics of stationary states*

- Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

##### *Non-equilibrium thermodynamic and hydrodynamic theories*

- Heavy ions in mixtures of light gases: Fokker-Planck equation and its solution, L. Ferrari 153 (1991) 115

*Ab initio schemes for stationary properties*

- Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1
- Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spiroonaterane, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
- Observable-dedicated molecular orbitals. I. Method and illustrations, J. Miralles, R. Caballol and J.-P. Malrieu 153 (1991) 25
- Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition, M. Raynaud, C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle 153 (1991) 39
- Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
- A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
- The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
- The magnetizability and g-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
- The structures and stability of the  $\text{Si}_3\text{H}_6^+$  dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
- Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the  $\text{CO}^{2+}$  case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
- Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
- The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409

*Computational and simulation methods*

- Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
- A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
- Trajectory capture rate coefficients for ion-quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
- Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
- The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409
- Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
- Electron spin exchange in micellized radical pairs. I.  $^{13}\text{C}$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}\text{C}$  radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
- Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
- Conformational dependence of the quadratic hyperpolarisabilities of a series of push-pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457

*Molecular dynamics and scattering theory*

- Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51

- Trajectory capture rate coefficients for ion-quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
- An extended diatomics-in-molecules model for  $\text{NH}_2^+$ , R. Polák 153 (1991) 91
- Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
- Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201
- Estimation of the integral cross section for dissociative excitation of  $\text{F}_2$  by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
- Experimental**
- Magnetic resonances*
- Electron spin exchange in micellized radical pairs. I.  $^{13}\text{C}$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}\text{C}$  radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
- Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
- Microwave spectroscopy*
- The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
- Visible and UV spectroscopy*
- Dissociative excitation of hydrogen in rf and dc glow discharges through  $\text{H}_2$ , S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
- Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of  $\text{CFCl}_3$ , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
- Multiphoton dissociation dynamics of highly excited states of  $\text{CS}_2$  and  $\text{CS}_2$  clusters, E. Patsilina, D. Proch and C. Fotakis 153 (1991) 503
- Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
- The  $\text{C}(^3\text{P}_j) + \text{NO}(X^2\Pi_r) \rightarrow \text{CN}(X^2\Sigma^+) + \text{O}(^3\text{P}_j)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519
- Emission of  $\text{Xe}: \text{N}(^2\text{P})$  collision complexes near the  $\text{N}(^2\text{P} \rightarrow ^2\text{D})$  lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
- Anomalous behaviour of the anticrossing density as a function of excitation energy in the  $\text{C}_2\text{H}_2$  molecule, Chem. Phys. 152 (1991) 293., P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539
- Fluorescence spectroscopy*
- Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247

- The  $C(^3P_J) + NO(X^2\Pi_r) \rightarrow CN(X^2\Sigma^+) + O(^3P_J)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthé 153 (1991) 519
- Photoelectron and Auger spectroscopy*
- Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
- Electron impact spectroscopy*
- The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
- Estimation of the integral cross section for dissociative excitation of  $F_2$  by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
- Production of the  $N_2(A^3\Sigma^+_u)$  metastable state by electron impact dissociative excitation of  $N_2O$ , S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
- Laser methods*
- Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
- Picosecond spectroscopy*
- Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
- Non-linear optical spectroscopy*
- Conformational dependence of the quadratic hyperpolarisabilities of a series of push-pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
- Synchrotron spectroscopies*
- The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
- Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259
- Time-resolved experiments*
- Production of the  $N_2(A^3\Sigma^+_u)$  metastable state by electron impact dissociative excitation of  $N_2O$ , S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
- Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
- Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
- Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465

*Mass spectrometry*

- Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Lecomte and J.C. Lorquet 153 (1991) 201
- Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of  $\text{CFCl}_3$ , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
- Multiphoton dissociation dynamics of highly excited states of  $\text{CS}_2$  and  $\text{CS}_2$  clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503

*Measurement of macroscopic variables*

- Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

**Objects****Bulk systems***Gases*

- Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
- Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
- Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351
- Emission of  $\text{Xe}:\text{N}(^2\text{P})$  collision complexes near the  $\text{N}(^2\text{P} \rightarrow ^2\text{D})$  lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531

*Supersonic beams*

- The  $\text{C}(^3\text{P}_J) + \text{NO}(X^2\Pi_r) \rightarrow \text{CN}(X^2\Sigma^+) + \text{O}(^3\text{P}_J)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthé 153 (1991) 519

*Liquid mixtures and solutions*

- The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
- Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247
- Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
- Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
- Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
- Electron spin exchange in micellized radical pairs. I.  $^{13}\text{C}$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}\text{C}$  radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
- Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443

*Crystals*

- Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371

*-mixed*

- Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511

*Polymers*

- Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305

*Semiconductors*

- Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

*Surfaces*

- Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259

*Low-dimensional materials*

- Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371

*Dielectrics*

- A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125
- Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465

*Plasmas*

- Dissociative excitation of hydrogen in rf and dc glow discharges through H<sub>2</sub>, S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233

*Biological systems*

- A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125

**Microscopic systems***Atoms*

- Relation between total energy and sum of orbital energies for neutral atoms, A. Nagy and N.H. March 153 (1991) 141
- Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161

*Molecules (neutral and ionic)*

- A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63



- Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79
- Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
- Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
- The structures and stability of the  $\text{Si}_3\text{H}_6^+$  dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
- The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidone and 2-hydroxypyrimidine, A. Leś and L. Adamowicz 153 (1991) 409
- Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511
- diatomic*
- Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1
- Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storzhev and M.L. Strekalov 153 (1991) 99
- Estimation of the integral cross section for dissociative excitation of  $\text{F}_2$  by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
- Dissociative excitation of hydrogen in rf and dc glow discharges through  $\text{H}_2$ , S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
- Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the  $\text{CO}^{2+}$  case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
- Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
- The  $\text{C}(^3\text{P}_j) + \text{NO}(X^2\Pi_r) \rightarrow \text{CN}(X^2\Sigma^+) + \text{O}(^3\text{P}_j)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthé 153 (1991) 519
- small polyatomics*
- Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spiroonaterane, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
- Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
- Trajectory capture rate coefficients for ion-quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
- An extended diatomics-in-molecules model for  $\text{NH}_2^+$ , R. Polák 153 (1991) 91
- On the Jahn-Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133
- The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
- The magnetizability and g-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
- Production of the  $\text{N}_2$  ( $A^3\Sigma_u^+$ ) metastable state by electron impact dissociative excitation of  $\text{N}_2\text{O}$ , S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283



- Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
- Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of  $\text{CFCl}_3$ , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
- Multiphoton dissociation dynamics of highly excited states of  $\text{CS}_2$  and  $\text{CS}_2$  clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503
- Anomalous behaviour of the anticrossing density as a function of excitation energy in the  $\text{C}_2\text{H}_2$  molecule, Chem. Phys. 152 (1991) 293., P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539
- aromatics*
- Conformational dependence of the quadratic hyperpolarisabilities of a series of push–pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457
- other large*
- Acrylonitrile versus allyl cyanide: the role of electronic conjugation in high electric field condition, M. Raynaud, C. Reynaud, Y. Ellinger, G. Hennico and J. Delhalle 153 (1991) 39
- Molecular aggregates*
- Emission of  $\text{Xe:N}(^2\text{P})$  collision complexes near the  $\text{N}(^2\text{P} \rightarrow ^2\text{D})$  lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531
- dimers*
- Multiphoton dissociation dynamics of highly excited states of  $\text{CS}_2$  and  $\text{CS}_2$  clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503
- Free radicals (including hydronium and muonium)*
- Theory of multi-quantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
- Theory of multi-quantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
- Quasiparticles (including excitons)*
- The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
- Defects and impurities*
- Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483
- Ions and charge carriers*
- Heavy ions in mixtures of light gases: Fokker–Planck equation and its solution, L. Ferrari 153 (1991) 115
- Xerographic dark discharge of PVK: TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
- Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

## Phenomena

### *Molecular structure*

- Observable-dedicated molecular orbitals. I. Method and illustrations, J. Miralles, R. Caballol and J.-P. Malrieu 153 (1991) 25
- The structures and stability of the  $\text{Si}_3\text{H}_8^+$  dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
- Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the  $\text{CO}^{2+}$  case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
- Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415

### *Vibrations and rotations of molecules*

- Vibrational structure of the solvated glycine zwitterion, J.S. Alper, H. Dothe and D.F. Coker 153 (1991) 51
- Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strekalov 153 (1991) 99
- The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
- Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473

### *Electronic structure and states*

- Theoretical study of the spectroscopy of the alkali oxides LiO, NaO, and KO, S.R. Langhoff, H. Partridge and C.W. Bauschlicher Jr. 153 (1991) 1
- Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spiroonoteraene, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
- The solvated electron in an electrolyte solution, V.D. Lakhno and O.V. Vasil'ev 153 (1991) 147
- The electronic states of the azines. IV. Pyrazine, studied by VUV absorption, near-threshold electron energy-loss spectroscopy and ab initio multi-reference configuration interaction calculations, I.C. Walker and M.H. Palmer 153 (1991) 169
- Estimation of the integral cross section for dissociative excitation of  $\text{F}_2$  by electron impact, D.C. Cartwright, P.J. Hay and S. Trajmar 153 (1991) 219
- Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
- The structures and stability of the  $\text{Si}_3\text{H}_8^+$  dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
- Bond formation between positively charged species. Non-adiabatic analysis and valence-bond model in the  $\text{CO}^{2+}$  case, N. Levasseur, Ph. Millie, P. Archirel and B. Levy 153 (1991) 387
- Heteronuclear transition metal diatomics: the bonding and electronic structure of ScNi, YNi, ScPd and YPd, K. Faegri Jr. and C.W. Bauschlicher Jr. 153 (1991) 399
- Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
- Emission of Xe:  $\text{N}(^2\text{P})$  collision complexes near the  $\text{N}(^2\text{P} \rightarrow ^2\text{D})$  lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531

### *Electric and magnetic properties*

- Heavy ions in mixtures of light gases: Fokker-Planck equation and its solution, L. Ferrari 153 (1991) 115
- A dipolar chain model for the electrostatics of transmembrane ion channels, M.B. Partenskii, M. Cai and P.C. Jordan 153 (1991) 125

- The magnetizability and *g*-factor surfaces of ammonia, S.P.A. Sauer, V. Špirko and J. Oddershede 153 (1991) 189
- Xerographic dark discharge of PVK:TNF photoconductive material, J.-Y. Moisan, B. André and R. Lever 153 (1991) 305
- Ferromagnetism of charge-transfer crystals, A.L. Tchougreeff and I.A. Misurkin 153 (1991) 371
- Electron spin exchange in micellized radical pairs. I.  $^{13}\text{C}$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}\text{C}$  radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
- Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
- Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465
- Molecular interactions*
- An extended diatomics-in-molecules model for  $\text{NH}_2^+$ , R. Polák 153 (1991) 91
- Relaxation cross sections for transfer of rotational angular momentum in a semiclassical approximation, A.V. Storozhev and M.L. Strelakov 153 (1991) 99
- The correlated molecular electrostatic potential and electric field of 2(1H)-pyrimidine and 2-hydroxypyrimidine, A. Leš and L. Adamowicz 153 (1991) 409
- The  $\text{C}(^3\text{P}_1) + \text{NO}(X^2\Pi_r) \rightarrow \text{CN}(X^2\Sigma^+) + \text{O}(^3\text{P}_1)$  reaction dynamics studied at 0.06 and 0.23 eV relative translational energy in pulsed crossed supersonic molecular beams, C. Naulin, M. Costes and G. Dorthe 153 (1991) 519
- Spectral bandshapes and intensities*
- On the Jahn-Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133
- Doppler-free radio frequency lineshape theory for a three-level system with three allowed transitions in presence of an IR pump, S. Ghoshal and A. Datta 153 (1991) 161
- Dissociative excitation of hydrogen in rf and dc glow discharges through  $\text{H}_2$ , S.B. Vrhovac, S.B. Radovanov, S.A. Bzenić, Z.Lj. Petrović and B.M. Jelenković 153 (1991) 233
- Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
- Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of  $\text{CFCl}_3$ , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491
- Coupling of electronic and nuclear motion*
- On the Jahn-Teller coupling of an orbital triplet with a vibrational doublet, E. Ghelichkhani and E.R. Grant 153 (1991) 133
- Energy transfer processes*
- Near- and non-resonant (VV) energy transfer between molecules dissolved in liquid krypton: a comparison with liquid argon, J.J. Andrew, D.C. McDermott, S.P. Mills and C.J.S.M. Simpson 153 (1991) 247
- Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259

*Molecular photophysical processes*

- Transient spectroscopy of triphenylmethane derivatives following subpicosecond irradiation, M.M. Martin, P. Plaza and Y.H. Meyer 153 (1991) 297
- Excitation and ionization of freon molecules. IV. Absolute oscillator strengths for the photoabsorption (6–200 eV) and the ionic photofragmentation (11.5–49 eV) of  $\text{CFCl}_3$ , W. Zhang, G. Cooper, T. Ibuki and C.E. Brion 153 (1991) 491

*Intramolecular dynamics*

- Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Le-comte and J.C. Lorquet 153 (1991) 201
- Anomalous behaviour of the anticrossing density as a function of excitation energy in the  $\text{C}_2\text{H}_2$  molecule, Chem. Phys. 152 (1991) 293., P. Dupré, R. Jost, M. Lombardi, P.G. Green, E. Abramson and R.W. Field 153 (1991) 539

*-vibrational energy redistribution (including vibrational dissociation)*

- Quantum effects in competitive unimolecular reactions, F. Remacle, M. Desouter-Le-comte and J.C. Lorquet 153 (1991) 201

*Luminescence spectra, yields and lifetimes*

- Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
- Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333

*Non-linear responses (including optical)*

- Conformational dependence of the quadratic hyperpolarisabilities of a series of push-pull diaryl acetylenes: an experimental and computational investigation, M. Barzoukas, A. Fort, G. Klein, A. Boeglin, C. Serbutoviez, L. Oswald and J.F. Nicoud 153 (1991) 457

*Multiphoton phenomena*

- Ab initio calculations on the one- and two-photon electronic transitions of cyclopentadiene, spiroonaterane, 1,4-cyclo-hexadiene, Dewar benzene, norbornadiene, and barrelene, V. Galasso 153 (1991) 13
- Theory of multiquantum optically detected ESR spectra of radical pairs. I. General theory. Resonances in parallel radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 313
- Theory of multiquantum optically detected ESR spectra of radical pairs. II. Resonances in perpendicular radio-frequency field, V.A. Morozov and A.B. Doktorov 153 (1991) 333
- Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473
- Multiphoton dissociation dynamics of highly excited states of  $\text{CS}_2$  and  $\text{CS}_2$  clusters, E. Patsilinakou, D. Proch and C. Fotakis 153 (1991) 503
- Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511

*Reactions (including dissociation)**-gas phase*

- Trajectory capture rate coefficients for ion-quadrupolar molecule reactions, I. Mendaš and P. Milutinović 153 (1991) 73
- Production of the  $N_2$  ( $A^3\Sigma^+_u$ ) metastable state by electron impact dissociative excitation of  $N_2O$ , S.M. Barnett, N.J. Mason and W.R. Newell 153 (1991) 283
- Theoretical study of the reaction of OH with HNO, M.R. Soto, M. Page and M.L. McKee 153 (1991) 415
- Emission of  $Xe:N(^2P)$  collision complexes near the  $N(^2P \rightarrow ^2D)$  lines, A.F. Vilesov, J. Wildt and E.H. Fink 153 (1991) 531

*-condensed phase*

- Electron spin exchange in micellized radical pairs. I.  $^{13}C$  low field chemically induced dynamic nuclear polarization (CIDNP) and  $^{13}C$  radio frequency stimulated nuclear polarization (SNP), I.A. Shkrob, V.F. Tarasov and E.G. Bagryanskaya 153 (1991) 427
- Electron spin exchange in micellized radical pairs. II. Magnetic field and magnetic isotope effects in multinuclear pairs, I.A. Shkrob, V.F. Tarasov and A.L. Buchachenko 153 (1991) 443
- Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

*-photochemical*

- A quantum chemical study on the alternative mechanisms of the thermal cis-trans isomerization of streptocyanines, T. Krossner and F. Dietz 153 (1991) 63
- Core excitation-induced photodesorption of molecular and fragment ions from CO adsorbates on metal surfaces, R. Treichler, W. Wurth, W. Riedl, P. Feulner and D. Menzel 153 (1991) 259

*Electron transfer*

- Resonant two-photon ionization of phenol in methylene chloride doped solid argon using 248 nm KrF laser and 254 nm Hg lamp radiation, a comparative study. The UV/VIS absorption spectrum of phenol radical cation, K. Kesper, F. Diehl, J.G.G. Simon, H. Specht and A. Schweig 153 (1991) 511

*Ionization (including Rydberg states)*

- The structures and stability of the  $Si_3H_6^{2+}$  dications. A theoretical study, T. Kudo and S. Nagase 153 (1991) 379
- Highly excited states of nitric oxide studied by high-resolution resonance-enhanced multiphoton ionization spectroscopy, Y. Luo, Y.D. Cheng, H. Ågren, R. Maripuu, W. Seibt, L. Öhlund, P. Ejeklint, B. Carman, K.Z. Xing, Y. Achiba and K. Siegbahn 153 (1991) 473

*Surface effects and catalysis*

- Kinetics of the reactions of intrinsic and phosphorus doped polycrystalline silicon with molecular chlorine, Z.H. Walker and E.A. Ogryzlo 153 (1991) 483

*Thermodynamic and transport properties*

- Heavy ions in mixtures of light gases: Fokker-Planck equation and its solution, L. Ferrari 153 (1991) 115
- Generalized Einstein relations for ions in molecular gases, A.D. Koutselos and E.A. Mason 153 (1991) 351

*Structure of solids and liquids*

Cluster structure in model electrolyte solutions, J.L.F. Abascal and P. Turq 153 (1991) 79

*Phase transitions*

Xerographic discharge of organic thermoplastic material, J.Y. Moisan, B. André, R. Lever and C. Servens 153 (1991) 465